

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 157 °C

Global applicability domain: Inside

Local applicability domain index: 7.94e-01

Confidence level: 6.31e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Bromacil</div> <div>Measured: 158</div> <div>Predicted: 157</div>	<div>Image not found</div> <div>Terbacil</div> <div>Measured: 176</div> <div>Predicted: 164</div>	<div>Image not found</div> <div>Isocil</div> <div>Measured: 159</div> <div>Predicted: 158</div>
<div>Image not found</div> <div>Ethotoin</div> <div>Measured: 94.0</div> <div>Predicted: 113</div>	<div>Image not found</div> <div>Mephénytoin</div> <div>Measured: 137</div> <div>Predicted: 144</div>	